

# Diffusion and multifractality at the metal-insulator transition

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## Abstract

We review the time evolution of wavepackets at the metal-insulator transition in two- and three-dimensional disordered systems. The importance of scale invariance and multifractal eigenfunction fluctuations is stressed. The implications of the frequency- and wavevector-dependence of the diffusion coefficient are compared with the results of numerical simulations. We argue that network models are particularly suited for the investigation of the dynamics of disordered systems.

## I. INTRODUCTION

The time evolution of wavepackets reflects clearly the localization properties of the eigenstates of a system. While in infinite metallic systems wavepackets spread indefinitely and take on a Gaussian shape for long times, diffusion is absent in localized systems and wavepackets stay in a finite region around their starting point. In fact, the consideration of the diffusion of wavepackets has been the starting point of the theory of localization in random media [1]. At the mobility edge between metallic and insulating behavior the time evolution of wavepackets will be intermediate between the two extreme cases discussed above. The dynamics of wavepackets can be described by a frequency- and wavevector-dependent diffusion coefficient  $D(q, \omega)$ . Its behavior has previously been studied in detail [2–4]. The diffusion coefficient exhibits two characteristic features. First, from the scale invariance of the conductance [5] follows that the conductivity and via the Einstein relation the diffusion coefficient are scale dependent in higher than two dimensions. Thus only in two dimensions there exists a finite limit of  $D(q, \omega)$  as frequency and wavevector tend to zero. Secondly, on short distances and frequencies the diffusion coefficient reflects the multifractal correlations within single eigenfunctions of the system [6].

In this paper we focus on the time evolution of wavepackets. While the same information is encoded in the frequency- and wavepacket-dependence of the diffusion coefficient, we concentrate on the time dependence of characteristics of wavepackets like their return probability, their moments, and their shape. Our purpose in doing so is twofold. On the one hand elucidate these discussions some of the crucial differences between time evolution in the diffusive regime and at the mobility edge. On the other hand can the time evolution of wavepackets directly been studied in numerical simulations of network models, allowing for a check of predictions of scaling theory.

The paper is organized as follows: we first summarize the scaling form of the diffusion coefficient  $D(q, \omega)$ . Next we present the time dependence of the moments, return probability, and shape of wavepackets that results from this scaling form. And finally, we compare these

predictions with numerical results obtain for network models.

## II. SCALING FORM OF THE DIFFUSION COEFFICIENT

In this section we will briefly review known results about the scaling form of the diffusion coefficient. For a more complete discussion see, e.g., refs. [2,4].

Consider the time evolution of a wavepacket that at time  $t = 0$  is localized as a  $\delta$ -function at the origin. Due to conservation of the probability the Fourier (Laplace) transform of its probability density with respect to space and time has of the form

$$P(q, \omega) = \frac{1}{-i\omega + D(q, \omega)q^2}. \quad (1)$$

A scaling form for  $D(q, \omega)$  that is consistent the conductance being scale invariant at the metal-insulator transition is

$$D(q, \omega) = \frac{\xi^{2-d}}{\hbar\rho} F(\xi/L_\omega, \xi q), \quad (2)$$

where  $\xi$  is the localization length,  $\rho = \rho(E)$  the density of states near the critical energy  $E = E_c$ ,  $F$  is a scaling function, and

$$L_\omega := (\rho\hbar\omega)^{-1/d} = L(\hbar\omega/\Delta)^{-1/d}, \quad (3)$$

is a third length scale, besides  $q^{-1}$  and  $\xi$ , relevant at the critical point ( $\Delta = (L^d\rho)^{-1}$  is the mean level spacing). At the critical point, where the localization length  $\xi$  diverges, the diffusion coefficient can be written as

$$D(q, \omega) = \frac{q^{d-2}}{\hbar\rho} f(qL_\omega). \quad (4)$$

From various limiting cases the following form of  $f(x)$  can be deduced:

$$f(x) = \begin{cases} c_\alpha \cdot x^{(2-d)/d} & : x \rightarrow 0 \\ c_\beta & : \text{for intermediate values of } x \\ c_\gamma \cdot x^{-\eta/d} & : x \rightarrow \infty \end{cases} \quad (5)$$

The behavior for large  $x$  is governed by multifractal density fluctuations in single eigenfunctions and the correlation exponent  $\eta$  is related to the generalized dimension  $D_2$  of the inverse participation ratio  $\eta = d - D_2$  [7]. Numerical support for this scaling form has previously been obtained from calculations of the two-particle spectral function and the wavepacket return probability of real-space and tight-binding models of the quantum Hall effect [8,3] as well as three-dimensional tight-binding models [4].

### III. SHAPE OF WAVEPACKETS

The shape of wavepackets  $P(r, t)$  can be obtained by transforming eq. (1) back to the space and time domain using the scaling form (5). The long time short distance behavior of  $P(r, t)$  is thus dominated by multifractal eigenfunction fluctuations characterized by the exponent  $\eta$ . The inverse Laplace transform with respect to  $\omega$  in the limit of  $q^d t / \hbar \omega \gg 1$  is [4]

$$P(q, t) \sim (q^d t)^{-D_2/d}. \quad (6)$$

The shape of the wavepackets is given by the Fourier transform of this expression. The short distance behavior,  $r^d \ll t / \hbar \rho$ , is thus a power law [9]

$$P(r, t) \sim t^{-D_2/d} r^{D_2-d}. \quad (7)$$

It should be noted that while this is the short distance behavior it can cover many decades for long times and hence describes completely the bulk of the wavepacket for long times.

It also follows from eq. (6) that the return probability  $P(r = 0, t)$  decreases as a power of time [3]

$$P(r = 0, t) \sim t^{-D_2/d}. \quad (8)$$

We notice that the shape of the wavepacket and hence the return probability depends of the generalized dimension  $D_2$  reflecting the influence of the multifractal eigenfunction fluctuations. In contrast to that, the moments of the probability distribution of a wavepacket

$m_k(t) = \int d^d r r^k P(r, t)$  do not depend on  $D_2$ . From the scaling form (5) it follows that  $P(q, t) = p(q^d t / \hbar \rho)$  and

$$m_k(t) = \int d^d r r^k P(r, t) = \Omega_d \int_0^\infty dr r^{d-1+k} \int \frac{d^d q}{(2\pi)^d} e^{-i\mathbf{q}\cdot\mathbf{r}} P(q, t), \quad (9)$$

$$= t^{k/d} \Omega_d \int_0^\infty dy y^{d-1+k} \int \frac{d^d x}{(2\pi)^d} e^{-i\mathbf{x}\cdot\mathbf{y}} p(x), \quad (10)$$

where  $x = q^d t / \hbar \omega$  and  $\Omega_d$  is the surface area of the  $d$ -dimensional unit sphere. The moments of the wavepacket are integral aspects of the shape of the wavepacket that are not dominated by its short distance behavior. Instead due to scale invariance they scale like  $t^{k/d}$ .

The behavior of wavepackets at the mobility edge should be contrasted to the well-known metallic behavior of asymptotically Gaussian wavepackets

$$P(r, t) = \frac{e^{-r^2/(4Dt)}}{(4\pi Dt)^{d/2}}, \quad (11)$$

with constant diffusion coefficient  $D$  and moments  $m_k(t) \sim t^{k/2}$ . The exponents at the critical point differ from these results in that a) the space dimension  $d$  is replaced by the generalized dimension  $D_2$  due to the multifractal fluctuations and b) the factor 2 is replaced by  $d$  reflecting the scale invariance of the conductance that gives rise to factors with exponents  $d - 2$  in the critical case.

It is further instructive to compare our results for the wavepacket dynamics at the mobility edge of a disordered system to those obtained for general quantum-mechanical systems. Under quite general assumptions it was shown that the return probability decays like  $t^{-\tilde{D}_2}$ , where  $\tilde{D}_2$  is the generalized dimension of the spectral measure or the energy dependent local density of states [10]. In the other hand, the exponent of the spatial decay of a wavepacket is given by  $D_2 - d$ , where  $D_2$  is the generalized dimension of the spatial dependence of the local density of states discussed above [9]. Finally, in the absence of multiscaling the moments of a wavepacket grow like  $t^{k\beta}$  with  $\beta = \tilde{D}_2/D_2$  [9]. Our results obtained above are a special case of these more general results. They depend only on a single exponent  $D_2$  since at the mobility edge the generalized dimensions of the spatial and spectral dependence of the local density of states are related to each other,  $D_q = d\tilde{D}_q$  [3,11]. The origin of this simplification

is the occurrence of a single relevant length scale  $L_\omega$  (eq. (3)), connecting the energy and length scales.

#### IV. NUMERICAL RESULTS

In order to numerically study the time evolution of wavepackets for a system defined by a Hamiltonian it is necessary to diagonalize at least the part of the spectrum containing the support of the wavepacket and to calculate the corresponding eigenstates. Alternatively, one can apply the time evolution operator  $\exp(-iHt/\hbar)$  to a wavepacket. Here the problem is that the kinetic and potential energy terms in the Hamiltonian do not commute so that a discretization in small timesteps and the use of an exponential decomposition is necessary [12,13]. In any case, the spectrum contains in general extended, critical, and localized states at the same time. It is therefore difficult to extract the dynamics at the critical point from any superposition of eigenstates of a finite system. Both of these problems can be avoided by investigating network models [14–16]. These models are defined by a unitary network operator  $U$  that can be interpreted as a time evolution operator [11]. The disorder as well as the energy of the system enters the network operator as parameters. By tuning the energy and disorder to their critical values the network operator describes a system at criticality with no contributions from localized or extended states. A discrete time evolution in such a system is obtained by repeatedly acting with the operator  $U$  on a network state  $\psi$ :

$$\psi(t) = U^t \psi(0), \tag{12}$$

with integer  $t$ . Since all eigenstates of  $U$  are critical it is possible to start the time evolution with a wavepacket maximally peaked at a single site. Again, for a Hamiltonian system this is impossible due to the presence of eigenstates with different localization properties in the spectrum, limiting the minimum size of a wavepacket.

In order to investigate the dependence on the dimensionality we study both two- and three-dimensional systems. The two-dimensional system is a network model proposed by

Chalker and Coddington as a model system exhibiting the integer quantum Hall effect [15]. It has only localized eigenstates except for states at the single energy in the center of a Landau level that are critical. The three-dimensional model consist of a stack of coupled Chalker-Coddington networks corresponding to a layered system in a strong magnetic field [17]. This system exhibits a true metal-insulator transition with extended and localized phases separated by a mobility edge with critical states.

The behavior of the moments of wavepackets is shown in figs. (1) and (2). For the quantum Hall system in fig. (1) the logarithm of  $m_k(t)^2/k$  is plotted versus  $\ln t$  for  $k = 2, 4, 6, 8$ . Note that in  $d = 2$  the behavior of the moments is the same in the diffusive as well as the critical regime. In contrast for the three-dimensional system the exponent is different in the critical regime,  $k/d$ , and in the diffusive regime,  $k/2$ . This is illustrated in fig. (2), where  $m_4(t)$  is plotted for various energies from the metallic regime (topmost curve) to the localized regime (bottom curve) with the critical regime with an exponent of  $4/3$  in between.

The decay of the return probability has already been studied in refs. [3,4] finding agreement with the expected exponent of  $D_2/d$ . Here we present results for the shape of wave packets in a two-dimensional network in fig. (3). The topology of the sample is a torus and the time is chosen such that the power law decay is observable up to half of the diameter of the system. The observed exponent of  $2 - D_2 \approx 0.44$  agrees well with previous calculations of  $D_2$  from other quantities.

## V. CONCLUSIONS

The time evolution of wave packets at the mobility edge of disordered systems differs from the diffusive evolution of wavepackets in good metals. The wavepackets spread for all times but their shape never becomes Gaussian. The origin of this behavior is the scale invariance of the conductance and the multifractal fluctuations of the local density of states. The latter dominate the short distance, long time behavior of wavepackets. The return probability decays like  $t^{-D_2/d}$  and the bulk of wavepacket has a power law shape  $\sim r^{D_2-d}$ .

The moments of a wavepacket depend only weakly on the multifractal fluctuations in that their growth exponent in time,  $k/d$ , does not depend on  $D_2$  while the prefactor does. That only a single multifractal exponent  $D_2$  occurs and not one for the spatial and one for the spectral structure of the local density of states, as is generally the case, can be interpreted as consequence of the existence of a single length scale  $L_\omega$  connecting energy and length scales.

The numerical study of the time evolution of wavepackets is most economically performed for network models compared to models defined by a Hamiltonian. The network models are defined by a unitary network operator that provides a natural discrete time evolution. The problem then reduces to repeated applications of the network operator. The results of the numerical calculations are in agreement with the scaling arguments and with numerical calculations based on different methods.

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## REFERENCES

- [1] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
- [2] J. T. Chalker, Physica A **167**, 253 (1990).
- [3] B. Huckestein and L. Schweitzer, Phys. Rev. Lett. **72**, 713 (1994).
- [4] T. Brandes, B. Huckestein, and L. Schweitzer, Ann. Physik **5**, 633 (1996).
- [5] E. Abrahams, P. W. Anderson, D. C. Liciardello, and V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).
- [6] F. Wegner, Z. Phys. B **25**, 327 (1976).
- [7] W. Pook and M. Janßen, Z. Phys. B **82**, 295 (1991).
- [8] J. T. Chalker and G. J. Daniell, Phys. Rev. Lett. **61**, 593 (1988).
- [9] R. Ketzmerick, K. Kruse, S. Kraut, and T. Geisel, (1997), cond-mat/9611006.
- [10] R. Ketzmerick, G. Petschel, and T. Geisel, Phys. Rev. Lett. **69**, 695 (1992).
- [11] B. Huckestein and R. Klesse, Phys. Rev. B **55**, R7303 (1997).
- [12] T. Kawarabayashi and T. Ohtsuki, Phys. Rev. B **51**, 10897 (1995).
- [13] T. Kawarabayashi and T. Ohtsuki, Phys. Rev. B **53**, 6975 (1996).
- [14] B. Shapiro, Phys. Rev. Lett. **48**, 823 (1982).
- [15] J. T. Chalker and P. D. Coddington, J. Phys. C **21**, 2665 (1988).
- [16] R. Klesse and M. Metzler, Europhys. Lett. **32**, 229 (1995).
- [17] J. T. Chalker and A. Dohmen, Phys. Rev. Lett. **75**, 4496 (1995).

# FIGURES

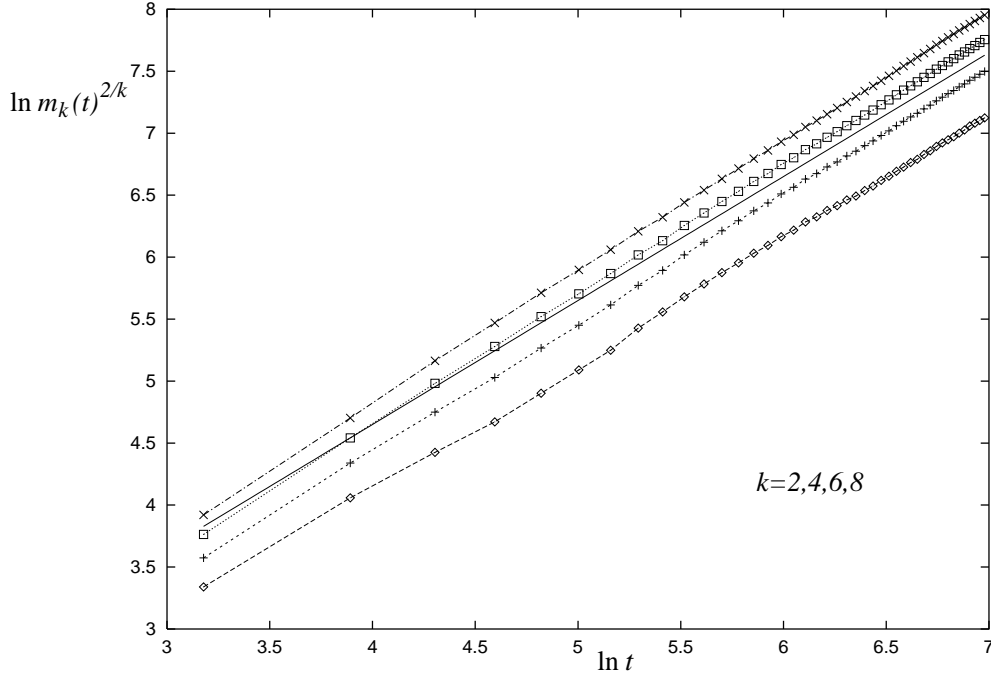


FIG. 1. Moments of a wavepacket  $m_k(t)^{2/k}$  versus time for a quantum Hall system and  $k = 2, 4, 6, 8$ .

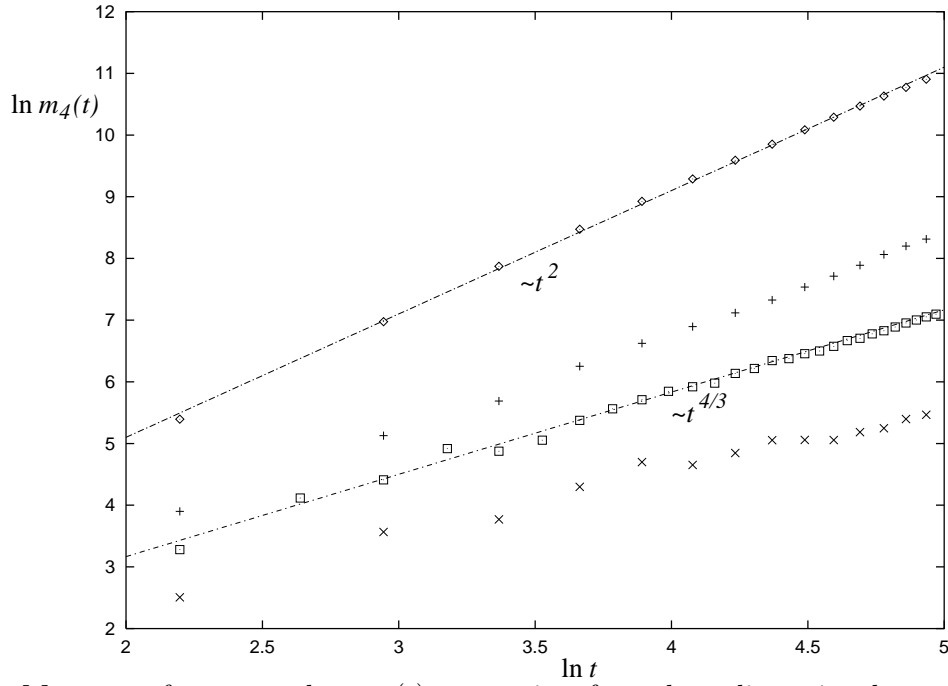


FIG. 2. Moments of a wavepacket  $m_k(t)$  versus time for a three-dimensional system and different energies showing diffusive (top), critical (center), and localized behavior (bottom).

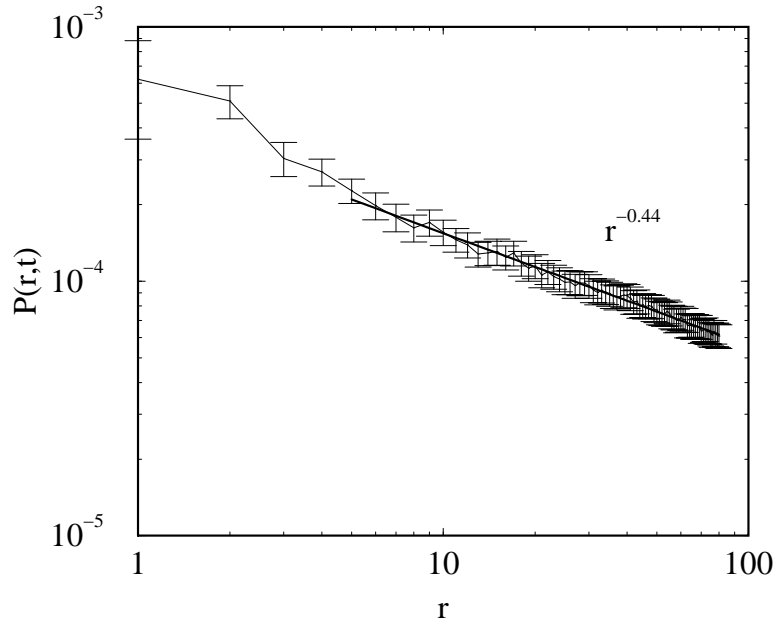


FIG. 3. Probability distribution  $P(r,t)$  of wavepackets for a quantum Hall system. The average over 5 different realizations of the disorder is shown. The size of the system is  $160 \times 160$  and double periodic boundary conditions are imposed.